

Cyclobutyl bromide

Other names:	Bromocyclobutane Cyclobutane, bromo-
Inchi:	InChI=1S/C4H7Br/c5-4-2-1-3-4/h4H,1-3H2
InchiKey:	KXVUSQIDCZRUKF-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	BrC1CCC1
Mol. weight [g/mol]:	135.00
CAS:	4399-47-7

Physical Properties

Property code	Value	Unit	Source
gf	45.77	kJ/mol	Joback Method
hf	-32.92	kJ/mol	Joback Method
hfus	7.44	kJ/mol	Joback Method
hvap	31.02	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.934		Crippen Method
mvol	73.860	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
tb	380.55 ± 0.60	K	NIST Webbook
tb	380.00 ± 3.00	K	NIST Webbook
tb	381.20	K	NIST Webbook
tc	580.15	K	Joback Method
tf	209.06	K	Joback Method
vc	0.271	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.92	J/mol×K	368.09	Joback Method
cpg	151.29	J/mol×K	544.80	Joback Method
cpg	143.62	J/mol×K	509.46	Joback Method
cpg	135.38	J/mol×K	474.12	Joback Method
cpg	126.54	J/mol×K	438.78	Joback Method

cpg	117.07	J/mol×K	403.43	Joback Method
cpg	158.44	J/mol×K	580.15	Joback Method
dvisc	0.0004717	Paxs	368.09	Joback Method
dvisc	0.0005432	Paxs	341.58	Joback Method
dvisc	0.0006405	Paxs	315.08	Joback Method
dvisc	0.0007786	Paxs	288.57	Joback Method
dvisc	0.0009844	Paxs	262.07	Joback Method
dvisc	0.0013122	Paxs	235.56	Joback Method
dvisc	0.0018813	Paxs	209.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4399477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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